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Coupled magnetic and molecular dynamics: Methodology and application to iron under high-pressure and temperature conditions

Wednesday 14 September 2022 11:30 (45 minutes)

Our presentation will first introduce a methodology aiming at simulating magneto-elastic phenomena. The approach is based on coupled classical spin dynamics and molecular dynamics. We will review the approach and its implementation in the LAMMPS code. After describing recent success of this methodology, we will point at some of its limitations.

We will then show how machine-learning interatomic potentials (ML-IAPs) trained on first-principles data, allowed us to circumvent some of those limitations. In particular, ML-IAPs were coupled to magneto-elastic spin Hamiltonians, altogether consistently trained on first-principles data.

Finally, we will display how the generated models can be used to simulate magneto-elastic phase transitions in iron, such as the Curie transition and its impact of thermophysical properties, the alpha to epsilon magneto-structural phase transition, or to perform high-pressure shock compression simulations.

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